

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.11

Global applicability domain: Inside

Local applicability domain index: 3.76e-01

Confidence level: 5.93e-01

Nearest Neighbors from the Training Set

[Image not found](#)

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Measured: 3.00

Predicted: 3.11

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5-Ethyl-1-methyl-5-(1-phenylethyl)pyrimidine-2,4,6(1H,3H,5H)-trione

Measured: 3.14

Predicted: 2.63